CONFORMATION-SPECIFIC SPECTROSCOPY OF JET-COOLED 4-PHENYL-1-BUTENE

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4-Phenyl-1-butene is the adduct formed by recombination of benzyl and allyl radicals, both of which are resonance-stabilized. Since resonance stabilized radicals build up in concentration under many conditions, formation of 4-phenyl-1-butene could be a preferred radical recombination pathway, analogous to propargyl recombination to form benzene. Unlike that latter reaction, 4-phenyl-1-butene has conformational flexibility, and its spectroscopic characterization thus benefits from conformation-specific methods. In this talk we report resonance-enhanced-two-photon ionization (R2PI), UV-UV hole-burning (UVHB), and rotational band contour (RBC) studies of 4-phenyl-1-butene. Three conformers were identified with their $S_1 \leftarrow S_0$ origins at 37525, 37528, and 37580 cm^{-1}. MP2 and DFT calculations predicted four low energy structures arising from anti or gauche arrangements about the Cα-Cβ bond and eclipsed (0°) or synclinal ($\pm 120^o$) vinyl group configurations about the Cβ-Cγ. The experimental rotational band contours were compared to simulated contours based on rotational constants and transition dipole moment directions as predicted by CIS calculations. Comparison allows for assignment of the bands to the gauche-synclinal+ (gs+), gauche-synclinal- (gs-), and anti-synclinal (as) structures, respectively.